

UNIVERSITY of WASHINGTON

CHEM LETTER

SUMMER 2015 / VOLUME XXXIII NO. 2

LETTER FROM THE CHAIR

Dear Friend of Chemistry,

Greetings from Michael Heinekey, as of July 1, the new occupant of the chair's office. In the last *ChemLetter*, former chair Paul Hopkins announced that he would be stepping down after an extraordinarily successful run of twenty years in office. Paul will be continuing with us as an outstanding teacher of organic chemistry.

As I write this, the UW administration is finalizing the budget for the coming biennium. As you may have heard, the legislature has voted to significantly increase the UW budget. For the first time in memory, our tuition for in-state undergraduates will actually *decrease*. After many years of steady increases which have significantly shifted the cost burden to students and their families, we are cautiously optimistic that a UW education may become more affordable.

The key to our academic success is the staff, faculty, and students that work together to discover and disseminate new developments in our discipline. We strive to recruit and retain the best candidates in all of these positions. I am very pleased to report that we have succeeded in recruiting Professor Anne McCoy from The Ohio State University. Anne is a very prominent theoretical/computational chemist who studies many fundamental aspects of molecular dynamics, especially the interpretation of vibrational spectral data resulting from large amplitude motions of transient species. A brief profile of Anne is found on page 4.

Undergraduate students in chemistry still learn the fundamentals of our discipline in ways familiar to earlier generations. The means for conveying this information is rapidly evolving, as shown by four Chemistry faculty members who were awarded the 2015 Distinguished Teaching Award for Innovation with Technology in a June ceremony at Meany Hall. Lecturers Jasmine Bryant and Colleen

Craig along with Assistant Professors AJ Boydston and Stefan Stoll were jointly recognized for their innovative use of technology in our instructional program. More about this very prestigious award is on page 5.

Recruiting of faculty is challenging, but turnover is relatively slow. In contrast, graduate students turn over much more rapidly and recruiting the best students is an ongoing challenge. One measure of the quality of our graduate students is the national competition for graduate research fellowships from the National Science Foundation. We have always encouraged our first-year students to submit proposals, but this process has been made more formal through the efforts of Assistant Professors AJ Boydston and David Masiello. AJ and David have organized a proposal writing course to guide the students in preparing competitive submissions. This has led to a steady increase in the number of successful proposals. This year, seven students received awards, with nine more receiving an honorable mention. The latter designation indicates that an outstanding proposal was submitted and would have been funded had more money been available. More about our fellowship winners can be found on pages 6-7.

I close with thanks to all of you for your generous contributions to the Department. Your gifts make possible many vital activities, including the recruiting of outstanding faculty and graduate students. We are very grateful for your generosity in giving back to today's students.

With best wishes,



D. Michael Heinekey
Professor and Chair

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CHEMICAL DYNAMICS AND THE RABINOVITCH LEGACY:

A SYMPOSIUM IN MEMORY OF B. S. RABINOVITCH



An excellent and engaging symposium on chemical dynamics was held here at the University of Washington on Saturday, May 30, 2015, to honor the memory of Professor Emeritus B. Seymour Rabinovitch and trace his scientific legacy. Rab, as we affectionately called him, passed away last year at the age of 95, and this symposium was a fitting tribute to his outstanding contributions.

Seven invited speakers from other institutions and two speakers from our department presented their latest results, providing a stimulating state-of-the-art overview of chemical dynamics research. The invited speakers included six members of the National Academy of Sciences, a Nobel Prize winner, and the current head of the Mathematical and Physical Sciences Directorate at the National Science Foundation: Emily A. Carter of Princeton University, F. Fleming Crim of the University of Wisconsin–Madison and NSF, Sharon Hammes-Schiffer of the University of Illinois at Urbana-Champaign, Stephen R. Leone of the University of California, Berkeley, David J. Nesbitt of the University of Colorado, Boulder, John C. Tully of Yale University, and Ahmed H. Zewail of the California Institute of Technology. The presentations by these world experts in the field of chemical dynamics informed the audience of the latest exciting developments in theory and experimental research in this area, stimulated much discussion, and will surely inspire future research.

Rab was one of the pioneers of chemical dynamics. His brilliant experiments performed during his four decades as a professor here provided most of our early quantitative measurements

of the efficiency with which energy is transferred between molecules in gas-phase intermolecular collisions and in collisions of molecules with solid surfaces. More importantly, his work provided quantitative estimates of the rates at which vibrational energy deposited locally within a molecule is redistributed amongst the many vibrational modes within that molecule. Rab's results proved that the equilibration of this vibrational energy almost always occurs within approximately one picosecond (10^{-12} s). He further showed that this validates (in most cases) the assumptions of RRKM Theory (Rice–Ramsperger–Kassel–Marcus Theory), and provided the first definitive examples where it breaks down. He also developed several widely used mathematical shortcuts for using RRKM Theory to make important predictions about physical chemistry. These shortcuts greatly increased both the applications and impact of RRKM Theory making it one of the most important theories of physical chemistry. It continues to guide much of our fundamental understanding of chemical dynamics and reaction kinetics even today. He received numerous highly prestigious awards for his scientific contributions, including the Peter Debye Award of the American Chemical Society and the Polanyi Medal of the Royal Society. He was a member of the American Academy of



(LEFT) B. S. RABINOVITCH AT THE BENCH IN THE MCGILL UNIVERSITY DEPARTMENT OF CHEMISTRY CIRCA 1939.

(CENTER) FLORA AND B. S. RABINOVITCH ON THE BURKE-GILMAN TRAIL, 2008.

(ABOVE) B. S. RABINOVITCH AT THE MACDONALD CHEMISTRY BUILDING, MCGILL UNIVERSITY, 1938.

Arts and Sciences and a Fellow of the Royal Society, London. He served as an editor for the *Journal of the American Chemical Society*, and was chairman of the Division of Physical Chemistry of the American Chemical Society. Forty-one students earned their Ph.D. under Rab's guidance; he counted them as lifelong friends.

In addition to being a great scientist, Seymour Rabinovitch was a wonderful husband and father. He raised four outstanding children, and later in life became an expert in the art of silversmithing, a writer of children's books, and a philanthropist. His offspring are following beautifully in his footsteps in their kindness to fellow human beings, their excellence in scholarship, science, and art, and their energetic dedication to improving the world through teaching, research, service, and philanthropy. The same can be said for his academic offspring as well.

We were honored to have 27 members of Rab's family attend the symposium, most notably his widow Flora, all four of his children, and their spouses and children. The family joined the speakers, many of our faculty, and some of Rab's former students and postdocs for a banquet after the symposium; it was tremendously enjoyable. Rab's daughter, Dr. Ruth Rabinovitch, and Professor Emeritus Alvin Kwiram gave touching tributes to his personal qualities and a summary of his life story and contributions to our department's growth.

The former chair of our department, Professor Paul Hopkins, referred to Rab as our "patriarch." Upon his passing, Paul wrote, "Through contribution, compounded by longevity, he gently exerted a powerful and extremely positive influence over this department. The quality of his scholarly work set a standard that each of us should aspire to match. Perhaps just as important, his kind and thoughtful manner, and commitment to diversity, contributed to the welcoming environment in this department that we all enjoy and benefit from to this day. Rab is gone now, but his contributions and influence live on."

It was a real honor for us to help organize this event in memory of this great man! We thank the Rabinovitch family and Paul Hopkins for asking us to organize it and for making it possible from a financial perspective, and we thank Diana Knight and the other staff from the front office for their kind and efficient logistical support.

Charles T. Campbell

Professor and B. Seymour Rabinovitch Endowed Chair in Chemistry

Munira Khalil

Associate Professor of Chemistry

FACULTY NEWS

Anne McCoy to Join Faculty

We are delighted to announce that Anne McCoy will be joining the Department as Professor of Chemistry for the 2015-16 academic year. Professor McCoy is moving to the University of Washington from Ohio State University, where she has been on the faculty since 1994. McCoy is a leader in the area of theoretical spectroscopy and dynamics. Her research focuses on the development of theoretical and computational approaches for understanding spectral signatures of large amplitude motions. She is particularly interested in molecules that are of atmospheric and astrochemical interest, and other species that exhibit large amplitude excursions from the minimum energy geometry even at low-levels of excitation. She collaborates extensively with experimental groups, and finds that such collaborations allow them to tease out physical insights from complicated experimental measurements. She looks forward to expanding her network of collaborators at the UW.



McCoy earned a B.S. in chemistry from Haverford College, and her Ph.D. in theoretical chemistry from the University of Wisconsin-Madison with Ned Sibert where her research focused on developing approximate approaches to study vibrational spectra. She then did postdoctoral work with R. Benny Gerber, dividing her time between the Hebrew University of Jerusalem and the University of California, Irvine. During that period, she developed approaches for applying quantum and classical dynamics to studies of photodissociation events in clusters. She joined the faculty at Ohio State in 1994, where she rose through the ranks.

Professor McCoy is deputy editor of the *Journal of Physical Chemistry A*, and she previously served as senior editor of the *Journal of Physical Chemistry*. She is a member of the American Chemical Society's Committee on Professional Training, which she chaired from 2012-2014. Professor McCoy's many honors include Ohio State University's Distinguished Scholar Award and Arts & Sciences Distinguished Faculty Award, several named lectureships, and election as a fellow of the American Physical Society, the American Chemical Society, and the American Association for the Advancement of Science.

McCoy is very excited about her move to the UW and is looking forward to getting settled in Seattle.

Look for a more detailed profile of Professor McCoy in a future issue of the *ChemLetter*.

Carroll, Li, and Maly Promoted

Congratulations to Lecturer Andrea Carroll on her promotion to Senior Lecturer and Associate Professors Xiaosong Li and Dustin Maly on their promotions to Professor, effective September 16, 2015.

Dr. Carroll joined the Department of Chemistry as a full-time lecturer in Autumn 2011 after having been an instructor in the general chemistry courses since Summer 2009. She has served as the general chemistry laboratory instructor, as well, since Autumn 2006, guiding the laboratory portion of the general chemistry series for approximately 3,000 students each year.

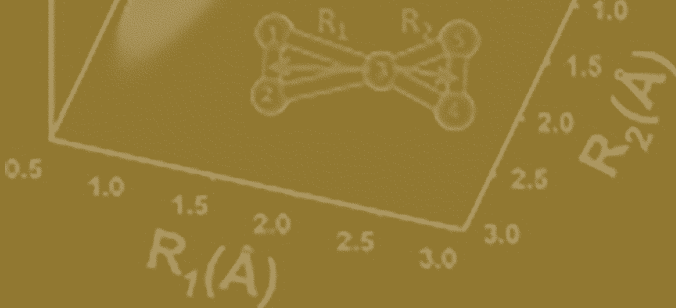


Professor Li's research focuses on the development of low-scaling methods to resolve excited state properties of many-electron systems, both in the time and frequency domains. This work is complimented by, and finds uses in, the development of efficient methods for studying non-adiabatic dynamics in large-scale systems.



Professor Maly is interested in developing new chemical tools that will allow a greater quantitative understanding of cellular signaling than is possible with currently available methods. Using the tools of organic synthesis they are generating cell permeable small molecules that allow the activation or inactivation of specific signaling enzymes in living cells.





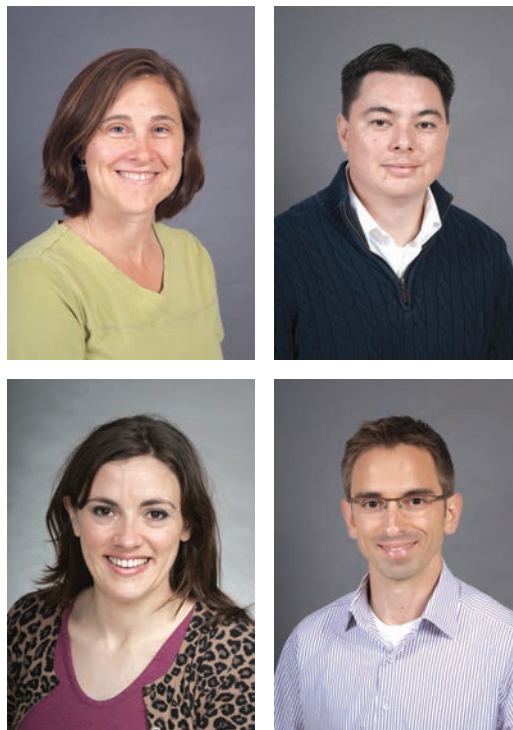
Chemistry Team Receives 2015 Distinguished Teaching Award for Innovation with Technology

A team of four Chemistry faculty members was awarded the 2015 Distinguished Teaching Award for Innovation with Technology. Lecturers Jasmine Bryant and Colleen Craig and Assistant Professors AJ Boydston and Stefan Stoll were jointly recognized for their innovative use of technology in our instructional program. They were honored with other 2015 Awards of Excellence recipients at a public ceremony on Thursday, June 11 in Meany Hall.

While the team members have each worked to improve student learning through technology in their individual courses, the overall impact has been broad. Their courses cover the range in our curriculum, from large undergraduate lecture courses in introductory general chemistry (Bryant, Craig) and organic chemistry (Boydston, Bryant) up to courses for our senior majors and graduate students (Stoll). Within Chemistry, the team serves as a resource for our faculty, piloting and vetting new technologies, advising our faculty on how best to adopt these technologies, generating a repository of modules, video mini-lectures, and tutorials shared among faculty, and making major contributions to curricular redesign. They have lowered the barrier for other faculty to make changes in their teaching, facilitating peer learning among colleagues in Chemistry as well as in other departments across campus. The efforts of all four are appreciated by the thousands of students they teach each year, who consistently reward their efforts with outstanding student course evaluation ratings.

Team members have been recognized for their experience and expertise in teaching at the local and national level. Bryant and Craig have participated in the Cottrell Scholars Collaborative National Teaching Assistant Workshop as well as a variety of teaching and learning initiatives at the UW, and Bryant received the 2013 "Most Engaging Lecturer" Award from the UW Panhellenic Association & Interfraternity Council. The Research Corporation for Science Advancement has honored Boydston (2014) and Stoll (2015) with the Cottrell Scholar Award, which recognizes 10-15 innovative early career teacher-scholars in chemistry, physics, and astronomy at U.S. institutions.

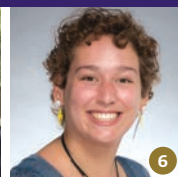
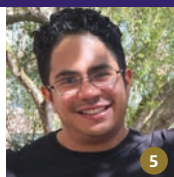
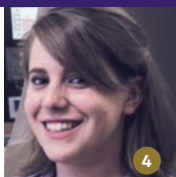
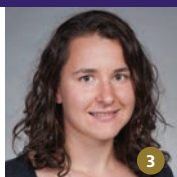
The University of Washington established the Distinguished Teaching Award in 1970 and five are awarded annually to faculty members from the Seattle campus. Recipients are chosen based on a variety of criteria, including mastery of the subject matter;



CLOCKWISE FROM TOP LEFT: JASMINE BRYANT, AJ BOYDSTON, STEFAN STOLL, COLLEEN CRAIG

enthusiasm and innovation in the teaching and learning process and in course and curriculum design; ability to inspire, guide, and mentor students through independent and creative thinking; and mentoring other faculty and teaching assistants to help enrich the scholarship of teaching and learning. Faculty members in Seattle who receive the Distinguished Teaching Awards are inducted into the UW Teaching Academy, where they will be able to participate in a variety of Academy-sponsored projects and events to further excellence in the teaching and learning process at the UW.

For more information about the 2015 Awards of Excellence, which honor UW achievements in teaching, mentoring, public service, and staff support, please visit washington.edu/facultystaff/awards.



SEVEN CHEMISTRY GRADUATE STUDENTS AWARDED

NSF GRADUATE RESEARCH FELLOWSHIPS

Congratulations to the seven graduate students in the Department of Chemistry who were awarded 2015 National Science Foundation Graduate Research Fellowships, and to the nine graduate students who received honorable mentions!

The NSF Graduate Research Fellowship Program recognizes and supports outstanding graduate students in NSF-supported science, technology, engineering, and mathematics disciplines who are pursuing research-based master's and doctoral degrees at accredited U.S. institutions. Fellows benefit from a three-year annual stipend along with a cost of education allowance for tuition and fees, opportunities for international research and professional development, and the freedom to conduct their own research at any accredited U.S. institution of graduate education they choose.

This year's large number of successful proposals from our students is, in part, due to the proposal writing course instituted by Assistant Professors AJ Boydston and David Masiello.

We hope you will enjoy learning about these gifted and hardworking students. In this issue, we introduce you to Rachel Eaton. Look for more profiles of fellowship recipients in future issues of the *ChemLetter*.

NSF GRADUATE RESEARCH FELLOWSHIP RECIPIENTS:

Rachel Eaton ❶

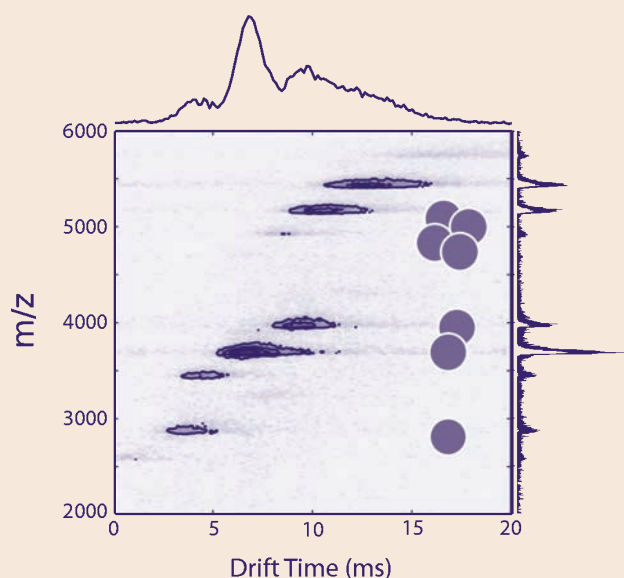
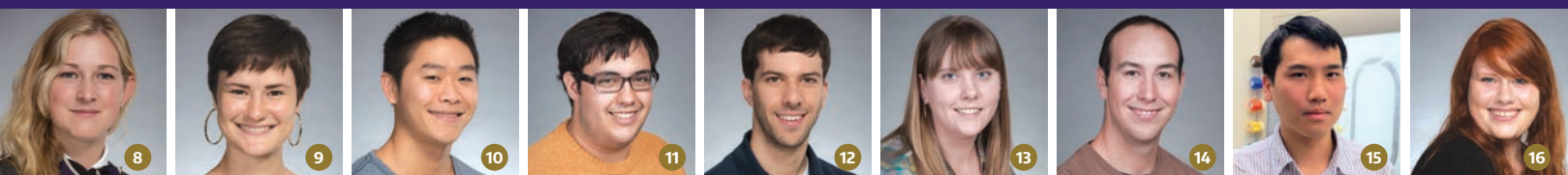
Advisor: Assistant Professor Matthew Bush

Rachel Eaton will be a second-year graduate student in the research group of Assistant Professor Matthew Bush. She uses ion mobility separation and mass spectrometry detection to analyze proteins and protein complexes in the gas phase. Ion mobility is a gas phase separation technique that works by guiding ions through a drift region filled with a known pressure of a gas such as N₂ or He. Traditionally, a stack of ring electrodes creates an electric field within the drift tube, such that ion velocity is determined by the opposing forces of the electric field propulsion and drag caused by collisions with drift gas molecules. This provides millisecond-scale, highly-resolved separations based on ion shape, size and charge. Coupling ion mobility to mass spectrometry detection (IM-MS) provides improved sensitivity and the ability to resolve the different charge states of an analyte. In particular, IM-MS is used in structural biology studies to determine the stoichiometry and shape of protein complexes.

Rae's work focuses on developing new ion mobility technology to improve and diversify large protein analysis. Currently, her work focuses on improving drift tube components with Structures for Lossless Ion Manipulation, or SLIM boards, developed by Dr. Richard Smith at Pacific Northwest National Laboratory. These SLIM boards are highly modular, and so non-linear drift regions become easier to fabricate and use in ion mobility experiments.

Using a combination of RF and DC potentials, ions are conducted through the drift region with minimal sample loss, providing an increased instrument sensitivity that is of particular importance in protein complex IM-MS analysis. In the accompanying figure (opposite page), concanavalin A was separated using a linear drift tube constructed from SLIM boards. Although each separation was





IM-MS ANALYSIS OF CONCAVALIN A SHOWING THE TETRAMERIC, DIMERIC, AND MONOMERIC CHARGE STATES. BOTH THE DRIFT TIME (ABOVE) AND M/Z (RIGHT) SPECTRA WERE ADDED TO EMPHASIZE RELATIVE PEAK INTENSITY.

milliseconds in length, a total acquisition time of a minute was used to increase signal intensity. As can be seen in the figure (above), the monomer, dimer, and tetramer forms of concanavalin A, as well as the charge states of each oligomeric state, were quickly resolved. Even within a short acquisition time, the SLIM boards showed improved sensitivity and resolution over traditional stacked ring electrodes. In the future, SLIM boards could be used to create an IMxIM-MS device with transmission rates not previously seen in protein complex samples. Such a device would allow us to probe low abundance proteins in more complex sample mixtures and to better study protein complexes that occur naturally at multiple oligomeric states.

Rae earned B.A. degrees in chemistry and biochemistry at Oberlin College, with a focus on bioanalytical chemistry. Her undergraduate research included work immobilizing liver microsomes for on-column LC-MS analysis of drug metabolites with Dr. Mark Parkin at Kings College London, and identifying and characterizing aptamer candidates for ovarian cancer biomarkers with Associate Professor Rebecca Whelan at Oberlin College. Though her family has lived in many places, her hometown is decidedly Portland, Oregon, and she accordingly likes hiking, DIY foodstuffs, and fiber arts.

Tyler Chozinski ²

Advisor: Assistant Professor Joshua Vaughan

"I owe my success to my determination and drive to master and overcome every challenge that stands between me and my yearning for knowledge."

Zuzana Culakova ³

Advisor: Professor Karen Goldberg

"My lifelong imperative to ask questions about the natural world has been the undercurrent of my love for chemistry."

Emily Dieter ⁴

Advisor: Associate Professor Dustin Maly

Marco Howard ⁵

Advisor: Assistant Professor Joshua Vaughan

"The public needs to hear about science in a context that is relevant and pertinent to their lives."

Johanna Schwartz ⁶

Advisor: Assistant Professor AJ Boydston

"Nothing is going to stop me or lessen my love of chemistry."

Karena Smoll ⁷

Advisor: Professor Karen Goldberg

HONORABLE MENTIONS:

Maike Blakely ⁸

Advisor: Professor Julie Kovacs

Caitlin Cornell ⁹

Advisor: Professor Sarah Keller

Andy Dang ¹⁰

Advisor: Professor František Tureček

"Growing up in a low-income immigrant household, health problems were common amongst my relatives; thus, enhanced quantitative tools for the advancement of biomedical assays are extremely important to me."

Michael De Siena ¹¹

Advisor: Professor Daniel Gamelin

Michael Enright ¹²

Advisor: Assistant Professor Brandi Cossairt

Lauren Gagnon ¹³

Advisor: Assistant Professor Joshua Vaughan

Troy Kilburn ¹⁴

Advisor: Professor Daniel Gamelin

Francis (Ray) Lin ¹⁵

Advisor: Professor Alex K.-Y. Jen

Chloe Lombard ¹⁶

Advisor: Associate Professor Dustin Maly

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GRADUATE PROGRAM NEWS *continued*

Gregory Peterson Awarded the Graduate Medal in the Natural Sciences

The College of Arts & Sciences annually names four graduate student medalists representing the four divisions of the College: Arts, Humanities, Social Sciences, and Natural Sciences. Gregory Peterson (Ph.D., Chemistry) was named the 2015 Graduate Medalist in the Natural Sciences. The following is reprinted from *Perspectives*, the College of Arts & Sciences newsletter:

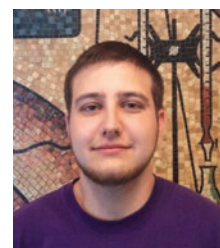
Gregory Peterson's passion for science comes through in his research as well as outreach projects for high school students.

His research focuses on polymers—large molecules composed of many repeated subunits. He has collaborated on several polymer-related research projects at the UW, including projects that may offer revolutionary capabilities in 3D printing. He has co-authored numerous papers about his work, and is included as an inventor on two patents being filed.

"Greg has been an invaluable component of my research group," says AJ Boydston, assistant professor of chemistry. "He has all the skills and makings of others I have seen go on to become scientific leaders at top academic institutions."

Peterson's impact extends to high school students. Through a collaboration with science faculty at Sammamish High School, he has developed problem-based STEM curriculum materials that offer a glimpse of what research can be. The curriculum has already benefited more than 750 students. Peterson has also developed and taught a lab course for incoming UW freshmen through the College of Engineering Bridge Program.

Peterson's next chapter? He will continue with chemistry research as a postdoctoral researcher at the University of Akron.



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Department of Chemistry, University of Washington

D. Michael Heinekey, Chair

Robert E. Synovec, Associate Chair for Graduate Education

Gary Drobny, Associate Chair for Undergraduate Education

Deborah Wiegand, Director of Entry-Level Programs

CONTRIBUTORS

Jasmine Bryant, Lecturer

Diana Knight, Assistant to the Chair
Creative Communications

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